

Understanding Ozone Pollution:

A Comparison of Chemical Mechanisms

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Motivation

- ▶ Importance of O_3 production chemistry representation – future emission scenarios.
- ▶ Compare O_3 chemistry representations used in photochemical modelling studies.
- ▶ Determine effects on O_3 production by comparing treatment of Volatile Organic Compounds (VOCs) degradation products.

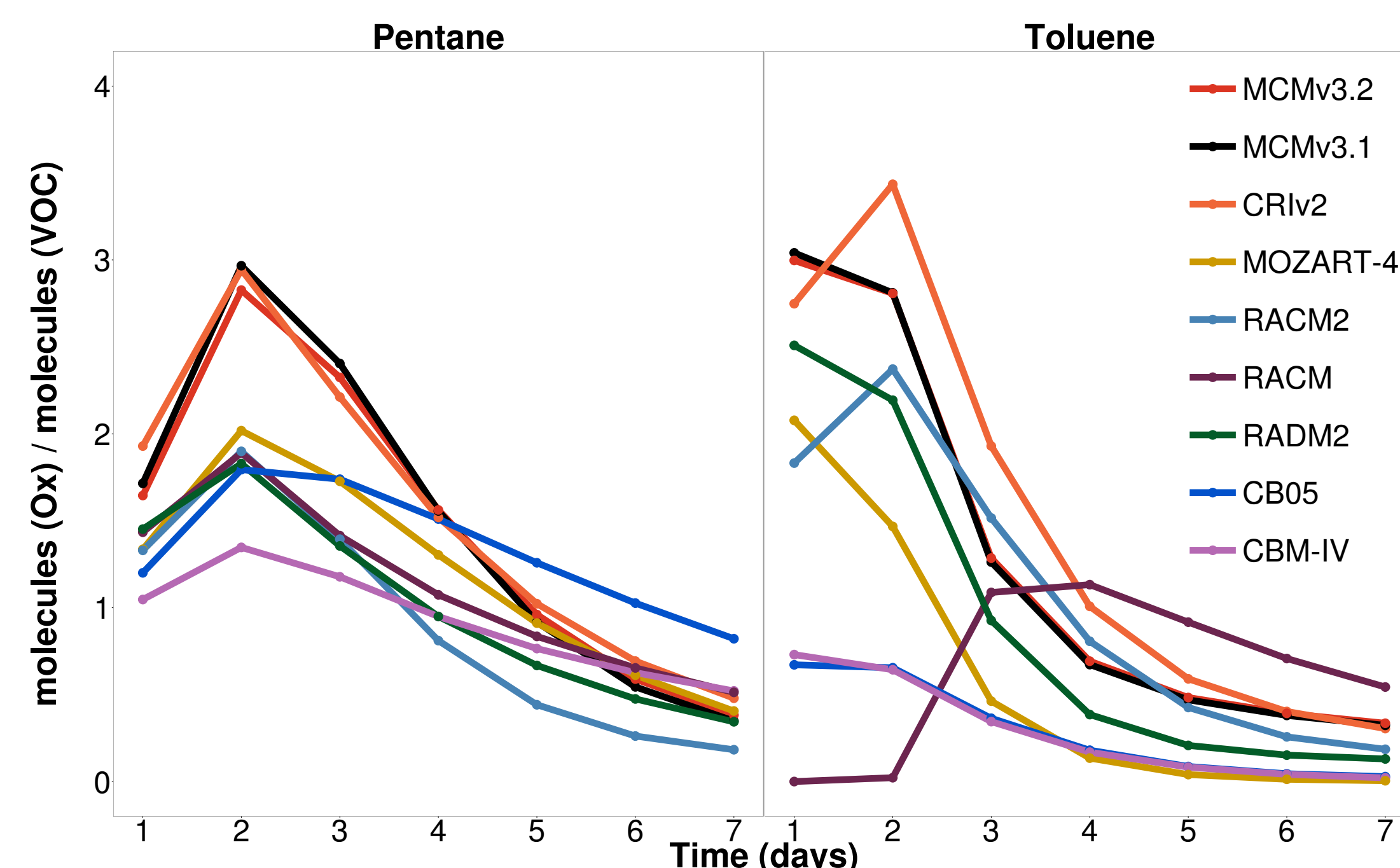
Approach

- ▶ Tagged Ozone Production Potentials (TOPPs) [1] calculated over 7 days for VOCs common to urban environments.
- ▶ Following mechanisms are compared to near-explicit MCM v3.2.

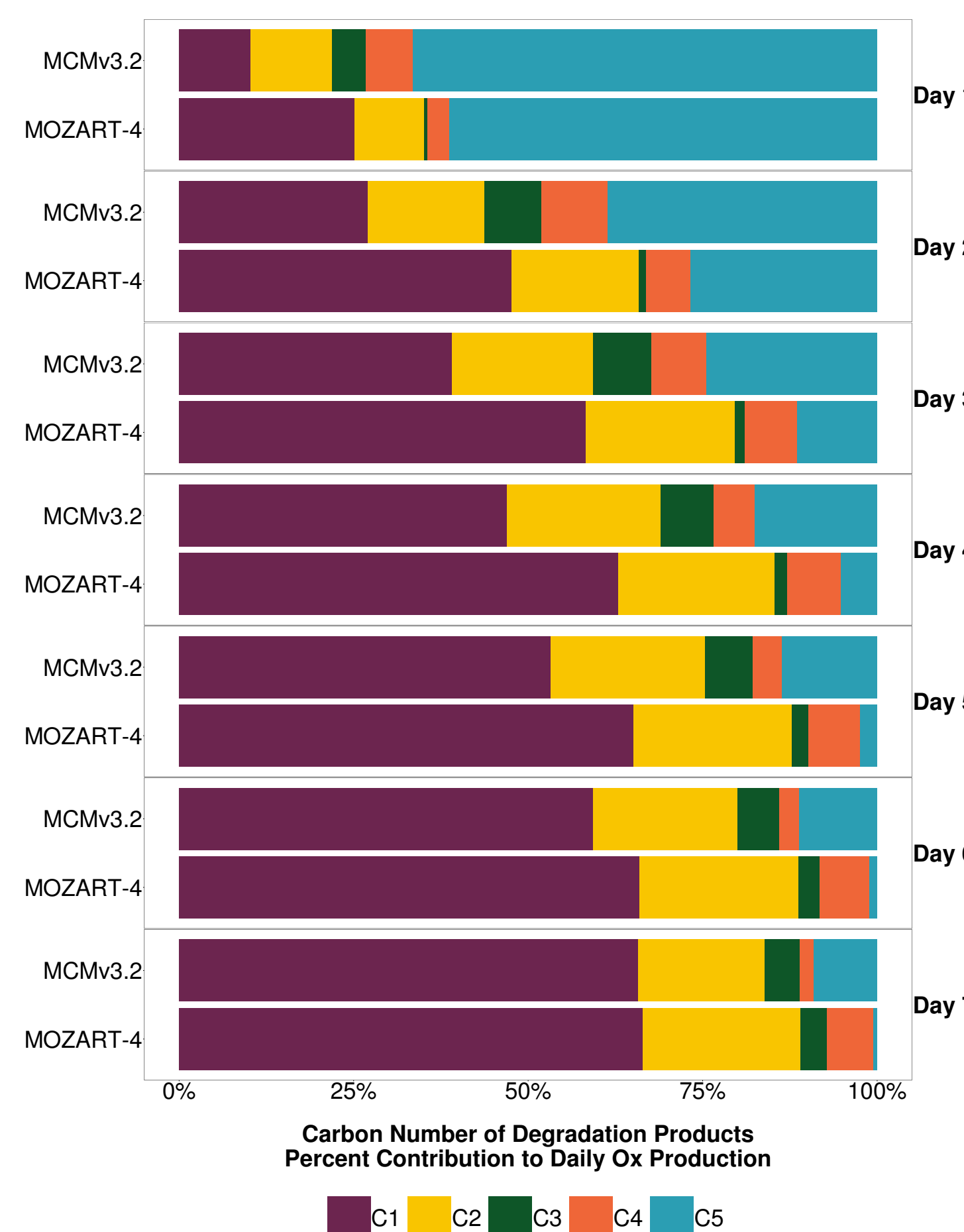
MCM v3.1	CRI v2	CBM-IV	CB05
RADM2	RACM	RACM2	MOZART-4
- ▶ O_x ($= O_3 + NO_2$) production allocated to emitted VOC by 'tagging' its organic degradation products.

Results

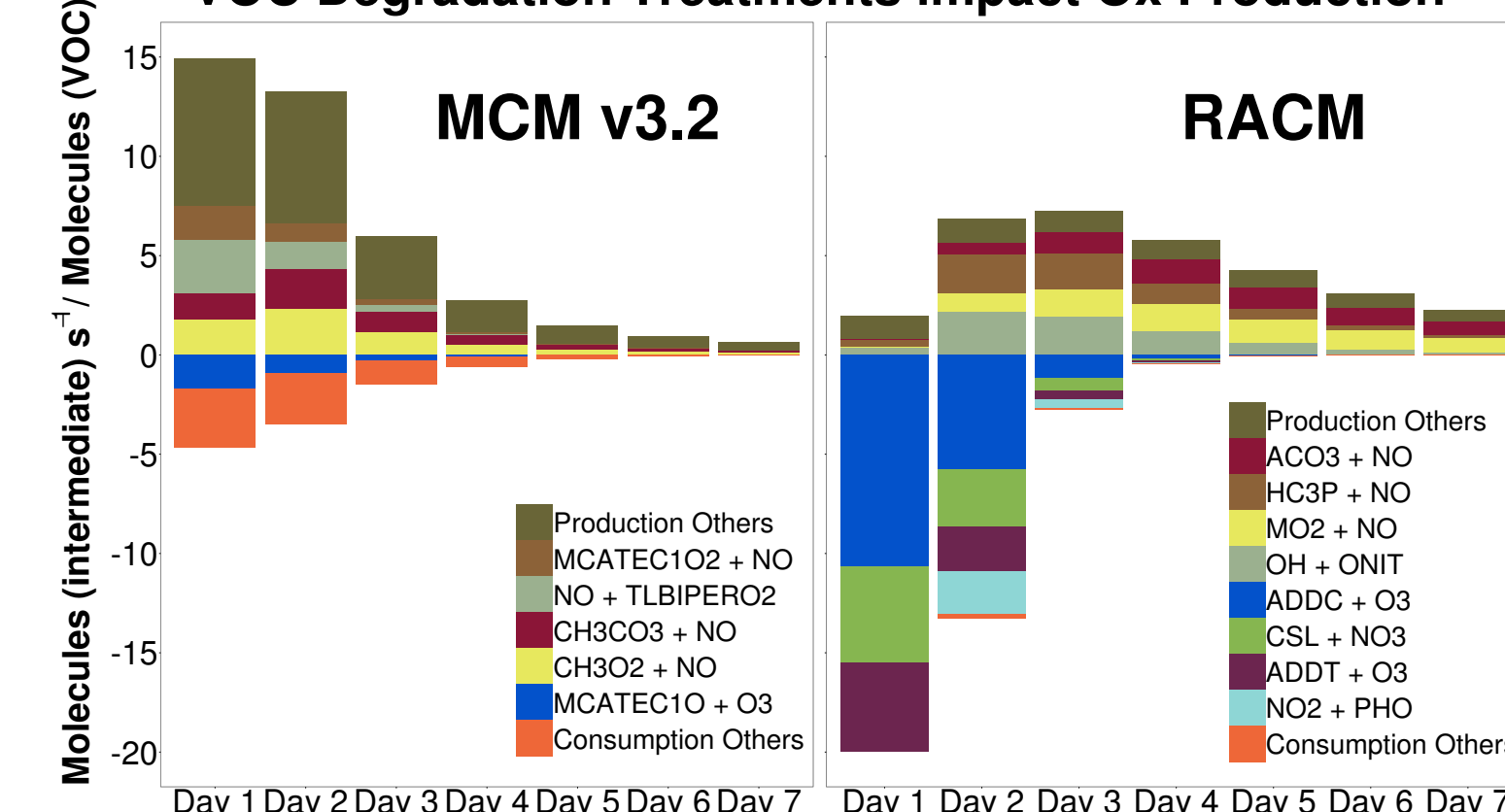
TOPP Time Series: Large Spread between Mechanisms



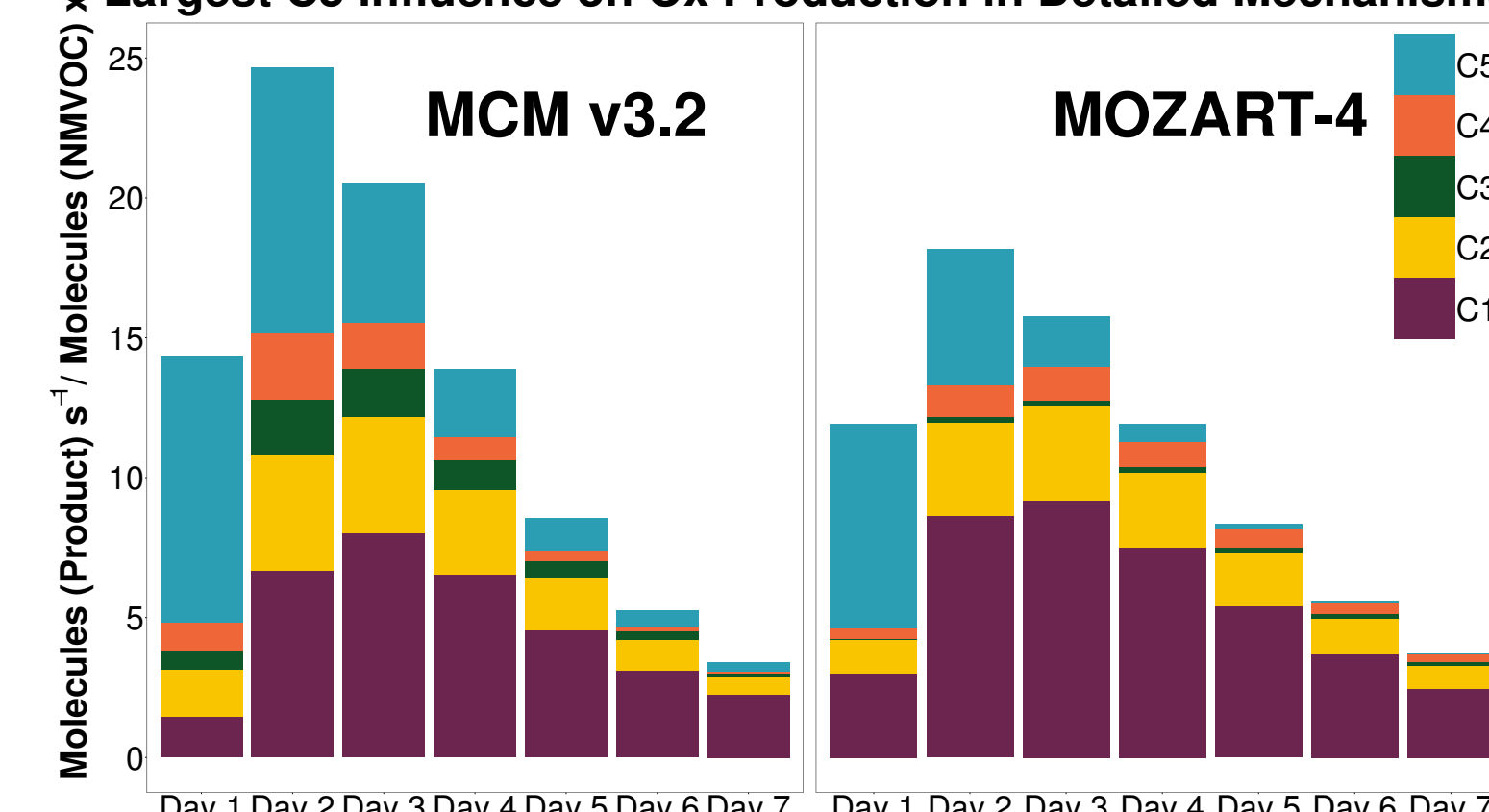
Pentane Relative Ox Production by Carbon Number:
Quicker VOC Break Down in Less-Explicit Mechanisms



Toluene Organic Ox Budgets:
VOC Degradation Treatments impact Ox Production



Pentane Absolute Ox Production by Carbon Number:
Largest C5 Influence on Ox Production in Detailed Mechanisms



Conclusions

- ▶ Near-explicit mechanisms produce more O_x than less-explicit mechanisms.
- ▶ VOCs broken down into smaller fragments quicker in less-explicit mechanisms resulting in less O_x production.
- ▶ Near-explicit mechanisms have highest influence of larger degradation products throughout.
- ▶ Differences in VOC degradation treatments impacts O_x production – RACM aromatic chemistry.

References

- [1] T. M. Butler, M. G. Lawrence, D. Taraborrelli, and J. Lelieveld. Multi-day ozone production potential of volatile organic compounds calculated with a tagging approach. Atmospheric Environment, 45(24):4082–4090, 2011.



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